Chapter 2
Setting, Hypotheses and Main Results

The overarching goal of this book is to propose an analytic-algebraic framework to make Linear Response Theory (LRT) rigorous for a wide class of systems. The purpose of this chapter is to explain the setting, enumerate the mathematical hypotheses and state the main results.

2.1 Description of the Abstract Setting

The first step for the construction of a general, and quite abstract setting for LRT is the introduction of the main ingredients.

Basic elements of the theory:

(H1) A *von Neumann algebra* $\mathscr{A} \subseteq \mathscr{B}(\mathcal{H})$ of bounded operators on the (not necessary separable) Hilbert space $\mathcal{H}$ which contains the relevant information about the system of interest. This von Neumann algebra is endowed with a *trace* $\mathcal{T}$ which allows us to compute expectation values of observables related to the system of interest.

(H2) A (possibly unbounded) selfadjoint Hamiltonian H *affiliated* to $\mathscr{A}$ which prescribes the *unperturbed* dynamics of the system.

(H3) A set $\{X_1, \dots, X_d\}$ of (possibly unbounded) selfadjoint operators, a vector $\boldsymbol{\Phi} \in \mathbb{R}^d$ of length $\Phi := |\boldsymbol{\Phi}|$ and a positive parameter $\varepsilon > 0$ which enter in the definition of a unitary-valued map $\mathbb{R} \ni t \mapsto G_{\Phi,\varepsilon}(t)$.

(H4) The latter has the role to define a time-dependent *adiabatic isospectral perturbation* by conjugating the Hamiltonian H with $G_{\Phi,\varepsilon}(t)$,

$$H_{\Phi,\varepsilon}(t) := G_{\Phi,\varepsilon}(t)\, H\, G_{\Phi,\varepsilon}(t)^*. \tag{2.1.1}$$

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(H5) An *instantaneous observable* described by a time-dependent (possibly unbounded) operator $\mathbb{R} \ni t \mapsto J(t)$, which models some relevant physical property of the system at time t.
(H6) A positive operator $\rho \in \mathscr{A}^+$ called (initial) *equilibrium state* which encodes the status of the system at $t = -\infty$.

The compatibility and the interplay between the elements listed above is guaranteed by a set of six hypotheses, one for each of the items above.

Remark 2.1.1 (Hypotheses of this work) Throughout this work *whenever we write "under the Hypotheses" we mean to impose Hypotheses 1–6 below.* Each of them enumerates the technical assumptions associated the to corresponding item in the list of basic elements, e.g. Hypothesis 1 stipulates the precise setting of (H1).

We reckon that some results may be proven under weaker or plainly different hypotheses, but since the overarching goal of this work is to provide a widely applicable and robust *framework* for LRT, we do not strive for utmost generality and deliberately aim to avoid unnecessary technical complications. ⋆

The first of these describes the relation between the von Neumann algebra and the trace in (H1):

Hypothesis 1 (Von Neumann algebra and trace) *The von Neumann algebra $\mathscr{A}$ is* semi-finite *and the trace $\mathcal{T}$ is* faithful*,* normal *and* semi-finite *(f.n.s.).*

Some basic facts about von Neumann algebras (including the notion of affiliation) and f.n.s. traces will be recalled in Sect. 3.1 while some concrete examples will be provided in Chaps. 4 and 7. Hypothesis 1 ensures the possibility of developing a "coherent" (non-commutative) integration theory over $\mathscr{A}$ (see Sect. 3.2). Such a trace allows for the construction of the Banach spaces $\mathfrak{L}^p(\mathscr{A})$ for all $1 \leqslant p < \infty$ as the "p-Schatten classes" associated to $\mathscr{A}$, and these Banach spaces are the analogue of the classical L^p-spaces. In particular, one has that $\mathfrak{L}^1(\mathscr{A}) \cap \mathscr{A} = \mathscr{A}_{\mathcal{T}}$ is the maximal domain (indeed an ideal) in $\mathscr{A}$ where the trace $\mathcal{T}$ is well-defined. The set of elements which are Hilbert-Schmidt with respect to $\mathcal{T}$ naturally form a Hilbert space $\mathfrak{L}^2(\mathscr{A})$ with scalar product $\langle\!\langle A, B \rangle\!\rangle_{\mathfrak{L}^2} := \mathcal{T}(A^* B)$, $A, B \in \mathfrak{L}^2(\mathscr{A})$. We point out that the spaces $\mathfrak{L}^p(\mathscr{A})$ *may contain also unbounded operators*, and here we see why the framework of von Neumann algebras is necessary if we want to go beyond bounded tight-binding operators (cf. Sect. 2.6 and Chap. 7). Indeed, the von Neumann algebra itself can be identified with $\mathfrak{L}^\infty(\mathscr{A}) = \mathscr{A}$, and we will often use this identification to simplify notation.

Because we admit *unbounded* Hamiltonians, H need not be an element of $\mathscr{A}$. Instead, it suffices if we make the following

Hypothesis 2 (Unperturbed Hamiltonian) $H \in \mathrm{Aff}(\mathscr{A})$ *is a selfadjoint operator on $\mathcal{H}$ that is* affiliated with *$\mathscr{A}$ (cf. Definition 3.1.3), where* $\mathrm{Aff}(\mathscr{A})$ *is the set of closed and densely defined operators affiliated to $\mathscr{A}$.*

Unfortunately, in all physically relevant situations in which H is unbounded the Hamiltonian H does not belong to any of the spaces $\mathfrak{L}^p(\mathscr{A})$ (see Remark 3.2.7), even though the $\mathfrak{L}^p(\mathscr{A})$ have unbounded elements. Nevertheless, thanks to the affiliation of H to $\mathscr{A}$ the time-evolution

$$\alpha_t^0(A) := \mathrm{e}^{-\mathrm{i}tH} A\, \mathrm{e}^{+\mathrm{i}tH}, \qquad t \in \mathbb{R},\ A \in \mathscr{A}, \tag{2.1.2}$$

generated by H often extends naturally to a one-parameter group of isometries ($\mathbb{R}$-flow) $\mathbb{R} \ni t \mapsto \alpha_t^0 \in \mathrm{Iso}\big(\mathfrak{L}^p(\mathscr{A})\big)$ on each of the $\mathfrak{L}^p(\mathscr{A})$ spaces. As a consequence of Proposition 3.2.16 the flow turns out to be *strongly continuous* on $\mathfrak{L}^p(\mathscr{A})$ in the sense that

$$\lim_{t \to t_0} \big\| \alpha_t^0(A) - \alpha_{t_0}^0(A) \big\|_p = 0 \qquad \forall A \in \mathfrak{L}^p(\mathscr{A}).$$

Standard arguments of the theory of C_0-groups on Banach spaces ensure that the dynamics α_t^0 on $\mathfrak{L}^p(\mathscr{A})$ is induced by a densely defined infinitesimal generator $\mathscr{L}_H^{(p)}$ called *p-Liouvillian* (see Sect. 5.1.1).

Consequence 2.1.2 (Unperturbed dynamics) *Suppose Hypotheses 1 and 2 hold true. Then the Hamiltonian H induces strongly continuous one-parameter group of isometries (an $\mathbb{R}$-flow)*

$$\mathbb{R} \ni t \mapsto \alpha_t^0 \in \mathrm{Iso}\big(\mathfrak{L}^p(\mathscr{A})\big)$$

for each, $1 \leqslant p < \infty$, which is called unperturbed dynamics. *Its generator $\mathscr{L}_H^{(p)}$, the p-*Liouvillian*, has a core $\mathfrak{D}_{H,p}^{00}$ (see Eq. (3.3.4)) where it acts as a generalized commutator,*

$$\mathscr{L}_H^{(p)}(A) = -\mathrm{i}\,[H, A]_\ddagger = -\mathrm{i}\,\big(H\,A - \big(H\,A^*\big)^*\big), \qquad A \in \mathfrak{D}_{H,p}^{00}.$$

We will study the unperturbed dynamics on $\mathfrak{L}^p(\mathscr{A})$ and its generator $\mathscr{L}_H^{(p)}$ in Sect. 5.1. The notion of *generalized commutator*

$$[A, B]_\ddagger := A\,B - \big(A^*\,B^*\big)^* \tag{2.1.3}$$

and of the domain $\mathfrak{D}_{H,p}^{00}$ will be described in Sect. 3.3.2.

The set of operators $\{X_1, \ldots, X_d\}$ described in (H3) is required to be compatible with the notion of integration induced by the trace $\mathcal{T}$ on the algebra $\mathscr{A}$. This fact is covered by the following

Hypothesis 3 ($\mathcal{T}$-compatible generators) *The selfadjoint operators $\{X_1, \ldots, X_d\}$ are* $\mathcal{T}$-compatible generators *in the sense that for all $k = 1, \ldots, d$ and for all $s \in \mathbb{R}$ they satisfy*

(i) $\mathrm{e}^{+\mathrm{i}sX_k}\, A\, \mathrm{e}^{-\mathrm{i}sX_k} \in \mathscr{A}$ *for all* $A \in \mathscr{A}$,

(ii) $\mathcal{T}\big(\mathrm{e}^{+\mathrm{i}sX_k}\, A\, \mathrm{e}^{-\mathrm{i}sX_k}\big) = \mathcal{T}(A)$ *for all* A *in the trace-ideal* $\mathscr{A}_{\mathcal{T}} \subset \mathscr{A}$, *and*

(iii) the $\{X_1, \ldots, X_d\}$ *are* strongly commuting, *i.e.*

$$\mathrm{e}^{+\mathrm{i}sX_j}\, \mathrm{e}^{+\mathrm{i}sX_k} = \mathrm{e}^{+\mathrm{i}sX_k}\, \mathrm{e}^{+\mathrm{i}sX_j}, \qquad \forall j, k = 1, \ldots, d.$$

We refer to the integer d *as the* dimension, *and to a common invariant core* $\mathscr{D}_{\mathrm{c}}$ *as* localizing domain.

This assumption allows to introduce ($\mathcal{T}$-compatible) *spatial derivations* on $\mathfrak{L}^p(\mathscr{A})$ as generators of an $\mathbb{R}$-flow,

$$\partial_{X_k}(A) := \lim_{s\to 0} \frac{\mathrm{e}^{+\mathrm{i}sX_k}\, A\, \mathrm{e}^{-\mathrm{i}sX_k} - A}{s}.$$

Formally at least, the $\partial_{X_k}(A)$ can be seen as commutators $\mathrm{i}\,[X_k, A]$. Evidently, these are densely defined on each $\mathfrak{L}^p(\mathscr{A})$ (see Sect. 3.4), and the associated gradient $\nabla := \big(\partial_{X_1}, \ldots, \partial_{X_d}\big)$ gives rise to (non-commutative) *Sobolev spaces*

$$\mathfrak{W}^{1,p}(\mathscr{A}) := \Big\{ A \in \mathfrak{L}^p(\mathscr{A}) \;\Big|\; \nabla(A) \in \mathfrak{L}^p(\mathscr{A}) \times \ldots \times \mathfrak{L}^p(\mathscr{A}) \Big\}.$$

The fact that the generators strongly commute (Hypothesis 3 (iii)) has several implications: First of all, it ensures the commutativity between the derivations ∂_{X_j}. Secondly, it guarantees the existence of a localizing domain $\mathscr{D}_{\mathrm{c}} \subset \mathcal{H}$ [75, Corollary 5.28]. Consequently, linear combinations $\lambda_1 X_1 + \cdots + \lambda_d X_d$ with $\lambda_1, \ldots, \lambda_d \in \mathbb{R}$ are essentially selfadjoint on $\mathscr{D}_{\mathrm{c}}$ and therefore extend to uniquely defined selfadjoint operators.

Hypothesis 3 also plays a key role in the definition of the family of unitary operators $G_{\Phi,\varepsilon}(t)$ which implement the adiabatic isospectral perturbation of the Hamiltonian via Eq. (2.1.1).

Hypothesis 4 (Adiabatic isospectral perturbations) *Let* $\boldsymbol{X} := (X_1, \ldots, X_d)$ *be the operator-valued vector made up of* $\mathcal{T}$*-compatible generators with localizing domain* $\mathscr{D}_{\mathrm{c}}$ *(cf. Hypothesis 3). We define the* switch function

$$s_\varepsilon(t) := \begin{cases} \mathrm{e}^{\varepsilon t} & t \leqslant 0 \\ 1 & t > 0 \end{cases}$$

with adiabatic rate $\varepsilon > 0$. *Consider a system of real-valued and continuous* modulation functions $f_k \in C(\mathbb{R})$, $k = 1, \ldots, d$, *which fulfill the following integrability condition*

$$\int_{-\infty}^{t} \mathrm{d}\tau\; s_\varepsilon(\tau)\, \big|f_k(\tau)\big| = \int_{-\infty}^{0} \mathrm{d}\tau\; \mathrm{e}^{\varepsilon t}\, \big|f_k(\tau)\big| + \int_{0}^{t} \mathrm{d}\tau\; \big|f_k(\tau)\big| < +\infty \qquad (2.1.4)$$

for all $t \in \mathbb{R}$ *and* $\varepsilon > 0$. *Given a* field $\boldsymbol{\Phi} := (\Phi_1, \ldots, \Phi_d) \in \mathbb{R}^d$ *define the vector valued functions* $\boldsymbol{f}^{\Phi}(t) := (\Phi_1 f_1(t), \ldots, \Phi_d f_d(t))$ *and* $\boldsymbol{\Phi}^{\varepsilon}(t) := (\Phi_1^{\varepsilon}(t), \ldots, \Phi_d^{\varepsilon}(t))$ *where*

$$\Phi_k^{\varepsilon}(t) := \int_{-\infty}^{t} \mathrm{d}\tau \; s_{\varepsilon}(\tau) \, f_k^{\Phi}(\tau) = \int_{-\infty}^{t} \mathrm{d}\tau \; s_{\varepsilon}(\tau) \, \Phi_k \, f_k(\tau). \tag{2.1.5}$$

Then (2.1.5) *implies* $\Phi_k^{\varepsilon} \in C^1(\mathbb{R})$ *and* $\lim_{t \to -\infty} \Phi_k^{\varepsilon}(t) = 0$. *The modulus* $\Phi := |\boldsymbol{\Phi}|$ *will be called the* field strength. *For each* $t \in \mathbb{R}$ *the operators*

$$F_{\Phi,\varepsilon}(t) := \boldsymbol{\Phi}^{\varepsilon}(t) \cdot \boldsymbol{X} = \sum_{k=1}^{d} \Phi_k^{\varepsilon}(t) \, X_k \,, \tag{2.1.6a}$$

$$\dot{F}_{\Phi,\varepsilon}(t) := s_{\varepsilon}(t) \, \boldsymbol{f}^{\Phi}(t) \cdot \boldsymbol{X} = s_{\varepsilon}(t) \sum_{k=1}^{d} \Phi_k \, f_k(t) \, X_k, \tag{2.1.6b}$$

are essentially selfadjoint on the core $\mathscr{D}_{\mathrm{c}}$, *and so extend to uniquely defined selfadjoint operators. The* adiabatic isospectral perturbations *associated to the generators* X_k, *the field components* Φ_k *and the modulations* f_k *is given by exponentiating* $F_{\Phi,\varepsilon}(t)$,

$$G_{\Phi,\varepsilon}(t) := \mathrm{e}^{+\mathrm{i} F_{\Phi,\varepsilon}(t)} = \prod_{k=1}^{d} \mathrm{e}^{+\mathrm{i} \Phi_k^{\varepsilon}(t) X_k}, \qquad t \in \mathbb{R}. \tag{2.1.7}$$

We refer to $\varepsilon \to 0$ *as the* adiabatic limit.

Notice that the second equality in (2.1.7) is just a consequence of the strong commutativity of the generators and the Trotter product formula [72, Theorem VII.31]. Hypothesis 4 is the "abstract" version of the perturbations used in [7, 49]. In case all modulations f_k are supported in $[t_0, +\infty)$ with $t_0 > -\infty$, one can fix t_0 as the *finite* initial time. Then one has $\Phi_k^{\varepsilon}(t) = 0$, and consequently $G_{\Phi,\varepsilon}(t) = \mathbb{1}$, for all $t \leqslant t_0$. Two situations will be particularly interesting for the aims of this work: The first one concerns the adiabatic switching of a *constant field* described by the conditions $f_1(t) = \cdots = f_d(t) = 1$ for all $t \in \mathbb{R}$. The second assumes that the switch function

$$f_k(t) = \int_{\mathbb{R}} \mathrm{d}\omega \; \mathrm{e}^{+\mathrm{i}\omega t} \; \hat{f}_k(\omega) \tag{2.1.8}$$

is smooth and that the perturbation is switched off at $t = +\infty$ again, i.e. it is the Fourier transform of $\hat{f}_k \in C_{\mathrm{c}}(\mathbb{R})$ which are assumed to be compactly supported and satisfy $\overline{\hat{f}_k(\omega)} = \hat{f}_k(-\omega)$ (so that the f_k are *real*-valued). Modulations with frequency expansions of the type (2.1.8) has been studied in [49] in the context of the derivation of the Mott formula for the ac-conductivity.

In view of Hypothesis 4 the perturbed Hamiltonian $H_{\Phi,\varepsilon}(t)$ defined by (2.1.1) possesses the two important properties (see Sect. 5.2.1), (1) *isospectrality*

$\mathrm{Spec}\big(H_{\Phi,\varepsilon}(t)\big) = \mathrm{Spec}(H)$ for all $t \in \mathbb{R}$, and (2) *affiliation* $H_{\Phi,\varepsilon}(t) \in \mathrm{Aff}(\mathscr{A})$ for all $t \in \mathbb{R}$. An isospectral perturbation $G_{\Phi,\varepsilon}(t)$ also induces an automorphism of the von Neumann algebra $\mathscr{A}$ given by

$$\gamma_t^{\Phi,\varepsilon}(A) := G_{\Phi,\varepsilon}(t)\, A\, G_{\Phi,\varepsilon}(t)^*, \qquad A \in \mathscr{A}. \tag{2.1.9}$$

Actions of this type extend to strongly continuous isometries on each of the Banach spaces $\mathfrak{L}^p(\mathscr{A})$ (again Proposition 3.2.16).

Consequence 2.1.3 (Existence of the interaction dynamics) *Suppose Hypotheses 1–3 hold, and let $t \mapsto G_{\Phi,\varepsilon}(t)$ be an adiabatic isospectral perturbation in the sense of Hypothesis 4. Then the prescription* (2.1.9) *induces a strongly continuous map of isometries*

$$\mathbb{R} \ni t \mapsto \gamma_t^{\Phi,\varepsilon} \in \mathrm{Iso}\big(\mathfrak{L}^p(\mathscr{A})\big)$$

for each $1 \leqslant p < \infty$ which is called interaction dynamics.

The properties of $\gamma_t^{\Phi,\varepsilon}$ are studied in Sect. 5.2.5. In particular, one has that

$$\|\cdot\|_p - \lim_{t\to-\infty} \gamma_t^{\Phi,\varepsilon}(A) = A = \|\cdot\|_p - \lim_{\Phi\to 0} \gamma_t^{\Phi,\varepsilon}(A) \qquad \forall A \in \mathfrak{L}^p(\mathscr{A}),$$

which means that $\gamma_t^{\Phi,\varepsilon}$ converges strongly to the identity map $\mathbb{1}_{\mathfrak{L}^p}$ at the initial time $t = -\infty$ and in the limit of vanishing perturbation $\Phi \to 0$. Moreover, in the case of regular elements $A \in \mathfrak{W}^{1,p}(\mathscr{A})$ one can differentiate (strongly) $\gamma_t^{\Phi,\varepsilon}$ in t obtaining

$$\frac{\mathrm{d}}{\mathrm{d}t}\gamma_t^{\Phi,\varepsilon}(A) = \gamma_t^{\Phi,\varepsilon}\Big(s_\varepsilon(t)\, \boldsymbol{f}^{\Phi}(t)\cdot\nabla(A)\Big) = \gamma_t^{\Phi,\varepsilon}\left(s_\varepsilon(t)\sum_{k=1}^{d} \Phi_k\, f_k(t)\, \partial_{X_k}(A)\right).$$

2.2 The Perturbed Dynamics: Bridge to Analysis

Ultimately, the core of LRT is a comparison between the interaction dynamics generated by the perturbation of H and the perturbed dynamics defined by $H_{\Phi,\varepsilon}(t)$ in the limit of small ε. The proof of the existence of a *unitary time propagator* $U_{\Phi,\varepsilon}(t,s)$ which implements the perturbed dynamics generated by $H_{\Phi,\varepsilon}(t)$ cannot be based on purely algebraic considerations, but requires the use of tools borrowed from functional analysis. For this reason we also need a set of technical assumptions about the interplay between the Hamiltonian H and the generators X_k.

To simplify the presentation of the next Hypothesis, let us introduce

$$\mathrm{ad}_{X_j}(H) := \mathrm{i}\,[X_j, H]$$

for the commutator of two suitable operators X_j and H. As usual, defining commutators of two potentially unbounded operators is fraught with technical problems, but that is something we will address below. It is tempting to identify $\mathrm{ad}_{X_j}(H)$ with $\partial_{X_j}(H)$, and while there are situations where the two coincide, we intentionally separate these two notions for reasons that we will elaborate upon in Sect. 3.4.1: in general it turns out that $\mathrm{ad}_{X_j}(H)$ needs to be defined as a functional analytic object whereas we consider ∂_{X_j} as an algebraic derivation on the Banach spaces $\mathfrak{L}^p(\mathscr{A})$ — and in many cases of interest we in fact have $H \notin \mathfrak{L}^p(\mathscr{A})$ (cf. Example 3.2.7).

The notation for κ_j-fold commutators simplifies to the compact expression

$$\mathrm{ad}_{X_j}^{\kappa_j} := \underbrace{\mathrm{ad}_{X_j} \circ \cdots \circ \mathrm{ad}_{X_j}}_{\kappa_j \text{ times}}$$

where by convention $\mathrm{ad}_{X_j}^0(H) := H$. Moreover, the fact that $\{X_1, \ldots, X_d\}$ commute leads to $\mathrm{ad}_{X_j} \circ \mathrm{ad}_{X_k} = \mathrm{ad}_{X_k} \circ \mathrm{ad}_{X_j}$ commuting amongst each other, and hence, we can use multiindex notation to simplify successive commutators with respect to different X_j's, namely

$$\mathrm{ad}_X^\kappa := \mathrm{ad}_{X_1}^{\kappa_1} \circ \cdots \circ \mathrm{ad}_{X_d}^{\kappa_d}$$

where $\kappa = (\kappa_1, \ldots, \kappa_d) \in \mathbb{N}_0^d$ and as usual $|\kappa| = \sum_{j=1}^d \kappa_j$. With this notation in hand, we can stipulate our hypothesis on the current operators.

Hypothesis 5 (Current expansion) *The selfadjoint Hamiltonian $H \in \mathrm{Aff}(\mathscr{A})$ and the set $\{X_1, \ldots, X_d\}$ of $\mathfrak{T}$-compatible generators with localizing domain $\mathscr{D}_\mathrm{c} \subset \mathcal{H}$ meet the following assumptions:*

(i) *The* joint core *$\mathscr{D}_\mathrm{c}(H) := \mathscr{D}_\mathrm{c} \cap \mathscr{D}(H)$ is a densely defined core for H and $X_k[\mathscr{D}_\mathrm{c}(H)] \subset \mathscr{D}_\mathrm{c}(H)$ for all $k = 1, \ldots, d$.*

(ii) *$H[\mathscr{D}_\mathrm{c}(H)] \subset \mathscr{D}_\mathrm{c}$ and the commutators*

$$J_\kappa := (-1)^{|\kappa|}\, \mathrm{ad}_X^\kappa(H), \qquad \kappa \in \mathbb{N}_0^d, \tag{2.2.1}$$

are essentially selfadjoint on $\mathscr{D}_\mathrm{c}(H)$, and therefore uniquely extend to selfadjoint operators (still denoted with the same symbol J_κ). With abuse of notation, we will also use $J_k := -\mathrm{ad}_{X_k}(H)$ in case of first-order current operators.

(iii) *Assume that there exists $N \in \mathbb{N}_0$ with*

$$J_\kappa = 0 \qquad \forall \kappa \in \mathbb{N}_0^d \text{ with } |\kappa| > N$$

on $\mathscr{D}_\mathrm{c}(H)$. The smallest such integer N is called the order of *H with respect to the family $\{X_1, \ldots, X_d\}$.*

(iv) *All the J_κ are infinitesimally H-bounded in the sense that for any $\delta > 0$ there are positive constants $a > 0$ and $\delta > b > 0$ such that*

$$\|J_\kappa \varphi\|_{\mathcal{H}} \leqslant a \ \|\varphi\|_{\mathcal{H}} + b \ \|H\varphi\|_{\mathcal{H}}\,, \qquad \forall\, \varphi \in \mathscr{D}_{\mathrm{c}}(H),$$

for all $\kappa \in \mathbb{N}_0^d$.

(v) The Hamiltonian H has a (possibly unbounded) spectral gap *marked by a real number $\xi \in \mathrm{Res}(H)$ in the resolvent set.*

Hypothesis 5, in its entirety, is quite strong and for this reason has several implications. Nevertheless many physical systems of interest fulfill the conditions listed above (see e.g. Chap. 7). Item (i) in Hypothesis 5 ensures that for all $t \in \mathbb{R}$ the perturbed Hamiltonians $H_{\Phi,\varepsilon}(t)$ are essentially selfadjoint on the common core $\mathscr{D}_{\mathrm{c}}(H)$ (see Lemma 5.2.1 (1)). In fact, it would be appropriate to call $\mathscr{D}_{\mathrm{c}}(H)$ localiz*ed* (as opposed to localiz*ing*) domain, but to better distinguish these two we will refer to it as joint domain instead.

Item (ii) is needed to unambiguously define the family of selfadjoint operator-valued tensors: the (unperturbed) *current density tensor*

$$\mathbf{J}^{(r)} := \big\{J_\kappa\big\}_{|\kappa|=r}, \qquad\qquad r = 1, \dots, N, \tag{2.2.2}$$

is the collection of all the

$$J_\kappa = \mathrm{i}^{\,|\kappa|}\Big[\Big[\big[[H, X_{k_1}]\,,\, X_{k_2}\big]\,,\, \dots\Big]\,,\, X_{k_r}\Big]$$

of order r where

$$\big(k_1, \dots, k_r\big) = \big(\underbrace{1, \dots, 1}_{\kappa_1 \text{ times}}\,,\, \dots\,,\, \underbrace{d, \dots, d}_{\kappa_d \text{ times}}\big)$$

are suitably repeated indices. The condition $H[\mathscr{D}_{\mathrm{c}}(H)] \subset \mathscr{D}_{\mathrm{c}}$ is essential to define these operators as generalized commutators in the sense of Definition 3.3.2. The conditions expressed in (i) and (ii) are also sufficient for the application of the *Baker–Campbell–Hausdorff formula* (in the generalized setting of [76, Sect. 2.11.B]) to the perturbed Hamiltonian $H_{\Phi,\varepsilon}(t)$. A straightforward calculation produces the relevant formula

$$H_{\Phi,\varepsilon}(t) = H + W_{\Phi,\varepsilon}(t) \tag{2.2.3}$$

which relates the isospectral perturbation of H to the *additive* perturbation $W_{\Phi,\varepsilon}(t)$. The latter can be expanded in function of the current densities (2.2.1) according to the formula

$$W_{\Phi,\varepsilon}(t) := \sum_{r=1}^{N} \frac{(-1)^r}{r!} \sum_{|\kappa|=r}^{d} w_\kappa^\varepsilon(t)\, J_\kappa \tag{2.2.4}$$

where the time dependent coefficients w_κ^ε are given in terms of (2.1.5) by

$$w_\kappa^\varepsilon(t) := \prod_{j=1}^{d} \Phi_j^\varepsilon(t)^{\kappa_j} \tag{2.2.5}$$

Formula (2.2.3), which provides the *current expansion* of the isospectral perturbation, is proved in Lemma 5.2.1 (2). At this stage it is appropriate to point out that, without further assumptions, the equality (2.2.3) makes sense only on the dense set $\mathscr{D}_{\mathrm{c}}(H)$. In order to extend this equality in a suitable and useful way one would ask that also the right-hand side of (2.2.3) is essentially selfadjoint on $\mathscr{D}_{\mathrm{c}}(H)$. This is exactly the role of item (iii) in Hypothesis 5 which allows for the application of the *Kato–Rellich Theorem* (see Lemma 5.2.1 (3) for the details). As a consequence one obtains that both sides of the (2.2.3) are essentially selfadjoint operators on $\mathscr{D}_{\mathrm{c}}(H)$ and so they define the same selfadjoint operator after taking the closure. Moreover, the domain of (2.2.3) (and therefore that of (2.1.1)) turns out to be independent of time,

$$\mathscr{D}\big(H_{\Phi,\varepsilon}(t)\big) = \mathscr{D}(H), \qquad \forall t \in \mathbb{R}. \tag{2.2.6}$$

Finally, item (iv) and the definition of $H_{\Phi,\varepsilon}(t)$ given by (2.1.1) ensure that also

$$\xi \in \mathrm{Res}\big(H_{\Phi,\varepsilon}(t)\big), \qquad \forall t \in \mathbb{R}, \tag{2.2.7}$$

lies in a spectral gap of $H_{\Phi,\varepsilon}(t)$. Properties (2.2.6) and (2.2.7), along with the regularity of the functions w_κ^ε in (2.2.5), ensure the existence of a *unitary* time propagator $U_{\Phi,\varepsilon}(t,s)$ which implements the perturbed dynamics generated by $H_{\Phi,\varepsilon}(t)$ (see Theorem 5.2.5). To some extent the propagator $U_{\Phi,\varepsilon}(t,s)$ is the main object of LRT, and Hypothesis 5 has the principal purpose of ensuring the existence of a $U_{\Phi,\varepsilon}(t,s)$ which is "regular enough" (in the sense of Proposition 5.2.5). As a matter of fact the mere existence of $U_{\Phi,\varepsilon}(t,s)$ can be deduced under weaker hypotheses than those stated in Hypothesis 5. However, Hypothesis 5 and especially the current expansion (2.2.3) are key ingredients to make LRT rigorous.

By construction $U_{\Phi,\varepsilon}(t,s) \in \mathscr{A}$ and so it can be used to define a dynamics on $\mathscr{A}$ by means of the prescription

$$\alpha^{\Phi,\varepsilon}_{(t,s)}(A) := U_{\Phi,\varepsilon}(t,s)\, A\, U_{\Phi,\varepsilon}(s,t), \qquad t,s \in \mathbb{R},\ A \in \mathscr{A}. \tag{2.2.8}$$

According to a standard argument (Proposition 3.2.16) this map extends to continuous family of isometries on each of the Banach spaces $\mathfrak{L}^p(\mathscr{A})$.

Consequence 2.2.1 (Existence of the perturbed dynamics) *Suppose Hypotheses 1–5 hold true. Let $U_{\Phi,\varepsilon}(t,s) \in \mathscr{A}$ be the unitary propagator generated by the isospectrally perturbed Hamiltonian $H_{\Phi,\varepsilon}(t)$. Then for each $1 \leqslant p < \infty$ the prescription* (2.2.8) *induces an isometry*

$$\mathbb{R} \times \mathbb{R} \ni (t,s) \mapsto \alpha^{\Phi,\varepsilon}_{(t,s)} \in \mathrm{Iso}\big(\mathfrak{L}^p(\mathscr{A})\big)$$

which is jointly strongly continuous in t and s. We refer to the mapping $(t, s) \mapsto \alpha^{\Phi,\varepsilon}_{(t,s)}$ *as the* perturbed dynamics.

The joint strong continuity of the perturbed dynamics $\alpha^{\Phi,\varepsilon}_{(t,s)}$ means that

$$\lim_{t\to t_0} \left\| \alpha^{\Phi,\varepsilon}_{(t,r)}(A) - \alpha^{\Phi,\varepsilon}_{(t_0,r)}(A) \right\|_p = 0 = \lim_{s\to s_0} \left\| \alpha^{\Phi,\varepsilon}_{(r,s)}(A) - \alpha^{\Phi,\varepsilon}_{(r,s_0)}(A) \right\|_p$$

for all $A \in \mathfrak{L}^p(\mathscr{A})$ and $r \in \mathbb{R}$. Moreover, this mapping is also a "perturbation" of the unperturbed dynamics α^0_t induced by H in the sense that

$$\lim_{\Phi\to 0} \left\| \alpha^{\Phi,\varepsilon}_{(t,s)}(A) - \alpha^0_{t-s}(A) \right\|_p = 0, \qquad \forall A \in \mathfrak{L}^p(\mathscr{A}),\ \forall t, s \in \mathbb{R},$$

independently of $\varepsilon > 0$. The last fact is just a consequence of the Duhamel formula (see Proposition 5.3.4 for the details). Properties of the perturbed dynamics $\alpha^{\Phi,\varepsilon}_{(t,s)}$ are investigated in full detail in Sect. 5.2.4.

Up to now, we have described three different types of dynamics on the space $\mathfrak{L}^p(\mathscr{A})$: the *unperturbed dynamics*, the *interaction dynamics* and the *perturbed dynamics*. All these maps can be used to define different time evolutions of the (initial) equilibrium state ρ enumerated in (H5). We are now in a position to state properly what "equilibrium" means.

Definition 2.2.2 (Initial equilibrium state) *Let* $H \in \mathrm{Aff}(\mathscr{A})$ *be a selfadjoint Hamiltonian. An* initial equilibrium state *for* H *is any positive element* $\rho \in \mathscr{A}^+$ *such that* $\alpha^0_t(\rho) = \rho$ *where* α^0_t *is the unperturbed dynamics generated by* H.

The first observation is that an initial equilibrium state is totally insensitive to the effect of the unperturbed dynamics. Therefore, one is most interested in the behavior of ρ under the interaction or perturbed dynamics. However, a careful analysis of the time evolution of the initial equilibrium state requires some extra regularity assumptions on ρ.

Hypothesis 6 (p-regular initial equilibrium state) *Let* ρ *be an initial equilibrium state in the sense of Definition 2.2.2. We will assume that* ρ *is* p-regular*, namely*

(i) $\rho \in \mathscr{A}^+ \cap \mathfrak{W}^{1,1}(\mathscr{A}) \cap \mathfrak{W}^{1,p}(\mathscr{A})$ *(*regularity*),*

(ii) $\rho \in \mathfrak{D}^{00}_{H,1} \cap \mathfrak{D}^{00}_{H,p}$ *(see Eq. (3.3.4)) and* $H\rho \in \mathfrak{W}^{1,1}(\mathscr{A}) \cap \mathfrak{W}^{1,p}(\mathscr{A})$ *(*H-regularity*), and*

(iii) $\partial_{X_k}(\rho) \in \mathfrak{D}^{00}_{H,1} \cap \mathfrak{D}^{00}_{H,p}$ *holds for all* $k = 1, \ldots, d$.

Item (i) also includes $\rho \in \mathfrak{L}^1(\mathscr{A}) \cap \mathfrak{L}^p(\mathscr{A})$ and the equilibrium condition immediately implies that $\rho \in \ker\left(\mathscr{L}^{(1)}_H\right) \cap \ker\left(\mathscr{L}^{(p)}_H\right)$ where $\mathscr{L}^{(p)}_H$ is the generator of α^0_t in $\mathfrak{L}^p(\mathscr{A})$. Item (ii) ensures that also $H\rho \in \mathfrak{L}^1(\mathscr{A}) \cap \mathfrak{L}^p(\mathscr{A})$. As a consequence of Proposition 5.1.3 one immediately gets that the equality

$$H\rho = (H\rho)^* \tag{2.2.9}$$

holds true in $\mathfrak{L}^1(\mathscr{A})$ and $\mathfrak{L}^p(\mathscr{A})$. Equation (2.2.9) is a kind of generalized commutation rule between ρ and H. In order to have a true commutation relation we need stronger assumptions that are not necessary for the moment. As a consequence of all the previous assumptions about the Hamiltonian H, the generators X_k and the initial equilibrium state one can prove that $J_k\,\rho \in \mathfrak{L}^1(\mathscr{A}) \cap \mathfrak{L}^p(\mathscr{A})$ and

$$H\,\partial_{X_k}(\rho) = J_k\,\rho + \partial_{X_k}(H\rho) \in \mathfrak{L}^1(\mathscr{A}) \cap \mathfrak{L}^p(\mathscr{A}) \tag{2.2.10}$$

for all $k = 1, \ldots, d$. Equality (2.2.10), which is proved in Lemma 6.1.1, will play a crucial role for the analysis of the perturbed dynamics of ρ. In particular (2.2.10) ensures that $H\,\partial_{X_k}(\rho) \in \mathfrak{L}^1(\mathscr{A}) \cap \mathfrak{L}^p(\mathscr{A})$ for all $k = 1, \ldots, d$. Let us point out that even though the conditions for ρ listed above seem to be quite strong, they are necessary and natural for the derivation of the Kubo formulas in the context of a LRT. For instance, Assumption 5.1 in [7] is equivalent (through [7, Proposition 4.2]) to the fact that ρ has to be 2-regular. Let us also mention that the condition $\rho \in \mathfrak{W}^{1,2}(\mathscr{A})$ was originally identified in [2] (see also [3]) as the main requirement for the derivation of the Kubo formula. Let us point out that a sufficient condition to construct an equilibrium state is to define $\rho := f(H)$ where f is any positive function in $L^\infty(\mathbb{R})$. In this way the equilibrium condition $\alpha_t^0(\rho) = \rho$ and the positivity condition $\rho \in \mathscr{A}^+$ are automatically satisfied. However, the class of positive function $\mathscr{S}^{1,p}_{\mathcal{T},X}(\mathbb{R}) \subset L^\infty(\mathbb{R})$ such that ρ verifies Hypothesis 6 relies strongly on the particular nature of the trace $\mathcal{T}$ and of the generators X_k. In many situations of physical interest the class $\mathscr{S}^{1,p}_{\mathcal{T},X}(\mathbb{R})$ is composed of functions with a sufficiently rapid decay at infinity (e.g. as the Schwartz functions in [7]). This aspect will be shortly discussed in Sect. 6.1.1.

An initial equilibrium state ρ is left invariant, by definition, under the unperturbed dynamics α_t^0. However it can be evolved by the interaction dynamics:

$$\rho_{\mathrm{int}}(t) \equiv \rho_{\mathrm{int}}(t;\varepsilon,\boldsymbol{\Phi}) := \gamma_t^{\boldsymbol{\Phi},\varepsilon}(\rho), \qquad t \in \mathbb{R}. \tag{2.2.11}$$

The state ρ can be evolved also by the perturbed dynamics $\alpha^{\boldsymbol{\Phi},\varepsilon}_{(t,s)}$ through the prescription

$$\rho_{\mathrm{full}}(t) \equiv \rho_{\mathrm{full}}(t;\varepsilon,\boldsymbol{\Phi}) := \lim_{s\to-\infty} \alpha^{\boldsymbol{\Phi},\varepsilon}_{(t,s)}(\rho), \qquad t \in \mathbb{R}, \tag{2.2.12}$$

seen as a limit in $\mathfrak{L}^1(\mathscr{A})$ and $\mathfrak{L}^p(\mathscr{A})$ according to the regularity of ρ. We refer to (2.2.12) as the *full* evolution of the initial state ρ. While *a priori* it is not at all clear whether this limit exists, under all these Hypotheses we can prove that the fully time-evolved state $\rho_{\mathrm{full}}(t)$ is indeed well-defined and it can be compared with $\rho_{\mathrm{int}}(t)$:

Theorem 2.2.3 (Comparison of the two dynamics) *Suppose Hypotheses 1–6 hold true, and let $r = 1$, p with p being the regularity degree of ρ from Hypothesis 6.*

(1) The limit which defines the full evolution $\rho_{\mathrm{full}}(t)$ given by (2.2.12) exists in $\mathfrak{L}^r(\mathscr{A})$, and can be expanded in terms of $\rho_{\mathrm{int}}(t)$, $\boldsymbol{\Phi}$, and the operator-valued vector

$$\mathbf{K}^{\Phi,\varepsilon}(t) := -\int_{-\infty}^{t} \mathrm{d}\tau \; s_\varepsilon(\tau)\, f_j(\tau)\, \alpha^{\Phi,\varepsilon}_{(t,\tau)}\big(\nabla\big(\rho_{\mathrm{int}}(\tau)\big)\big) \tag{2.2.13}$$

so that

$$\rho_{\mathrm{full}}(t) = \rho_{\mathrm{int}}(t) + \boldsymbol{\Phi} \cdot \mathbf{K}^{\Phi,\varepsilon}(t). \tag{2.2.14}$$

(2) The full evolution $t \mapsto \rho_{\mathrm{full}}(t)$ is the unique solution of

$$\begin{cases} \dfrac{\mathrm{d}\rho_{\mathrm{full}}}{\mathrm{d}t}(t) = -\mathrm{i}\big[H_{\Phi,\varepsilon}(t)\,,\ \rho_{\mathrm{full}}(t)\big]_{\ddagger} \\ \lim\limits_{t\to-\infty} \rho_{\mathrm{full}}(t) = \rho \end{cases} \tag{2.2.15}$$

where the limit and the derivative are taken in $\mathfrak{L}^r(\mathscr{A})$, and the generalized commutator $[\,\cdot\,,\,\cdot\,]_{\ddagger}$ is defined in (2.1.3).

The proof of this theorem can be found in Sect. 6.1.2. Let us point out that Theorem 2.2.3 is nothing more than an "abstract" generalization of [7, Theorem 1.1].

2.3 Linear Response and the Kubo Formula

In order to completely specify the context of LRT and to present the different incarnations of the Kubo-formula we need to discuss the role of (H4) in the initial list, i.e. the instantaneous observable $t \mapsto J(t)$. The prototypical observables which enter in the LRT are the current density tensors $\mathbf{J}^{(r)}$ given in (2.2.2). As $\mathbf{J}^{(r)}$ is generated by the unperturbed Hamiltonian H through iterated commutators, in the same way one can consider *instantaneously* perturbed current density tensors generated by the perturbed Hamiltonian $H_{\Phi,\varepsilon}(t)$. This leads to a family of operator-valued tensors

$$\mathbb{R} \ni t \mapsto \mathbf{J}^{(r)}_{\Phi,\varepsilon}(t) := G_{\Phi,\varepsilon}(t)\, \mathbf{J}^{(r)}\, G_{\Phi,\varepsilon}(t)^*$$

which are well-defined if one assumes the validity of Hypotheses 3 and 5 (cf. Sect. 6.2.1). This relevant type of instantaneous observables possesses some peculiar properties (Proposition 6.2.4) which are sufficient to derive the Kubo-formula. This motivates the attempt to generalize the family of instantaneous observable suitable for the LRT.

Definition 2.3.1 (Current-type observable) *Suppose Hypotheses 1–6 hold true. We say a time-dependent observable $\mathbb{R} \ni t \mapsto J_{\Phi,\varepsilon}(t)$ is of* current-type *with respect to $H_{\Phi,\varepsilon}(t)$ and ρ if the following holds:*

(i) $J_{\Phi,\varepsilon}(t)$ is an instantaneous perturbation, i.e. there exists a selfadjoint operator $J \in \mathrm{Aff}(\mathscr{A})$ with

$$J_{\Phi,\varepsilon}(t) := G_{\Phi,\varepsilon}(t) J G_{\Phi,\varepsilon}(t)^*, \qquad \forall t \in \mathbb{R}.$$

(ii) $J_{\Phi,\varepsilon}(t)\,\rho_{\mathrm{full}}(t) \in \mathfrak{L}^1(\mathscr{A})$ *for all* $t \in \mathbb{R}$ *and*

$$\lim_{t\to-\infty} J_{\Phi,\varepsilon}(t)\,\rho_{\mathrm{full}}(t) = J\rho$$

in the topology of $\mathfrak{L}^1(\mathscr{A})$.

(iii) $\mathscr{D}(H) \subseteq \mathscr{D}(J)$ *which in turn ensures* $J\,\frac{1}{H-\xi} \in \mathscr{A}$ *(cf. Lemma 3.3.7 (2)) and*

$$J_{\Phi,\varepsilon}(t)\,\frac{1}{H_{\Phi,\varepsilon}(t)-\xi} = \gamma_t^{\Phi,\varepsilon}\left(J\,\frac{1}{H-\xi}\right)$$

for all $t \in \mathbb{R}$.

The central quantity for LRT is the *macroscopic net current*

$$\mathscr{J}^{\Phi,\varepsilon}[J,\rho](t) := \mathcal{T}\Big(J_{\Phi,\varepsilon}(t)\,\big(\rho_{\mathrm{full}}(t) - \rho_{\mathrm{int}}(t)\big)\Big) \tag{2.3.1a}$$

$$= \mathcal{T}\big(J_{\Phi,\varepsilon}(t)\,\rho_{\mathrm{full}}(t)\big) - \mathcal{T}(J\rho) \tag{2.3.1b}$$

associated to the initial equilibrium state ρ, evolved using the full evolution (2.2.15), and the current-type observable J. As a difference of expectation values this quantity measures the net flow of the *macroscopic* current between the fully evolved state $\rho_{\mathrm{full}}(t)$ and the "dragged along" state $\rho_{\mathrm{int}}(t)$. Because we slowly switch on the perturbation field $\boldsymbol{\Phi}$ at rate $\varepsilon > 0$, heuristically we expect $\rho_{\mathrm{full}}(t) \approx \rho_{\mathrm{int}}(t)$ to hold in case ε is small. For the precise justification of the second equality (2.3.1b) we refer to Sect. 6.2.1. Item (ii) in Definition 2.3.1 ensures the *equilibrium condition*, i.e. zero net flux in the distant past,

$$\lim_{t\to-\infty} \mathscr{J}^{\Phi,\varepsilon}[J,\rho](t) = 0.$$

We will elaborate on this further in Remark 6.2.3. Moreover, under all the Hypotheses listed above we will prove in Lemma 6.2.1 the absence of net current

$$\lim_{\Phi\to 0} \mathscr{J}^{\Phi,\varepsilon}[J,\rho](t) = 0$$

in the limit of vanishing perturbations. Consequently, the first term in the "Taylor expansion" of $\mathscr{J}^{\Phi,\varepsilon}[J,\rho](t)$ around $\boldsymbol{\Phi} = 0$ vanishes, and the first non-trivial term in

$$\mathscr{J}^{\Phi,\varepsilon}[J,\rho](t) = \sum_{k=1}^{d} \Phi_k\,\sigma_k^{\varepsilon}[J,\rho](t) + \mathcal{O}(\Phi^2). \tag{2.3.2}$$

describes the *linear response* of the system to the perturbation. Mathematically speaking, our task is to ensure that $\mathscr{J}^{\Phi,\varepsilon}[J,\rho](t)$ is sufficiently regular in the fields — mere continuity does not suffice. These first-order corrections are collectively known as the *conductivity coefficients*.

Definition 2.3.2 (Conductivity coefficients) *Let ρ by an initial equilibrium state for the Hamiltonian $H \in \mathrm{Aff}(\mathscr{A})$ and J a current-type observable. The ε-dependent* conductivity coefficients *generated by perturbing the system adiabatically at rate $\varepsilon > 0$ via a field $\boldsymbol{\Phi}$ between the initial time $-\infty$ and the final time t, is the d-dimensional vector with components*

$$\sigma_k^{\varepsilon}[J,\rho](t) := \frac{\partial}{\partial \Phi_k} \mathscr{J}^{\Phi,\varepsilon}[J,\rho](t)\Big|_{\Phi=0}, \qquad k = 1,\dots,d,$$

when they exist. Their adiabatic limits

$$\sigma^k[J,\rho] := \lim_{\varepsilon\to 0^+} \sigma_k^{\varepsilon}[J,\rho](t), \qquad k = 1,\dots,d,$$

are also referred to as conductivity *or* Kubo coefficients *whenever they exist.*

We are now in position to state the main result.

Theorem 2.3.3 (The Kubo formula) *Suppose that in addition to Hypotheses 1–6 we are given a current-type observable $J(t)$ in the sense of Definition 2.3.1. Then the ε-dependent conductivity coefficients are given by the* Kubo formula

$$\sigma_k^{\varepsilon}[J,\rho](t) = -\mathrm{i}\int_{-\infty}^{t} \mathrm{d}\tau\; s_{\varepsilon}(\tau)\, f_k(\tau)\, \mathcal{T}\left(J\, \alpha_{t-\tau}^0\left(\partial_{X_k}(\rho)\right)\right) \tag{2.3.3}$$

for each $k = 1,\dots,d$ where the f_k are the modulation functions from Hypothesis 4.

The proof of this result is postponed to Sect. 6.2.2. By inserting the explicit expression for the switch function s_{ε} into (2.3.3) we can rewrite the conductivity coefficients

$$\sigma_k^{\varepsilon}[J,\rho](t) = \widetilde{\sigma}_{\varepsilon}^k[J,\rho](t) + \delta_{\varepsilon}^k[J,\rho](t) \tag{2.3.4}$$

as the sum of two terms, a non-trivial contribution,

$$\widetilde{\sigma}_{\varepsilon}^k[J,\rho](t) := -\mathrm{i}\,\mathrm{e}^{\varepsilon t}\,\mathcal{T}\left(\int_0^{+\infty} \mathrm{d}\tau\; \mathrm{e}^{-\varepsilon\tau}\; f_k(t-\tau)\; J\; \alpha_{\tau}^0\big(\partial_{X_k}(\rho)\big)\right), \tag{2.3.5}$$

and a remainder which vanishes in the adiabatic limit (cf. Lemma 6.3.1),

$$\lim_{\varepsilon\to 0^+} \delta_{\varepsilon}^k[J,\rho](t) = 0.$$

In view of the fact that we are interested in the adiabatic limit, the last observation allows us to consider the quantity $\widetilde{\sigma}_{\varepsilon}^k[J,\rho](t)$ instead of $\sigma_k^{\varepsilon}[J,\rho](t)$. The following

result uses that the Laplace transform relates the evolution automorphism α_τ^0 and the resolvent of the Liouvililan on $\mathfrak{L}^p(\mathscr{A})$,

$$\frac{1}{\mathscr{L}_H^{(p)} + \varepsilon}(A) = \int_0^{+\infty} \mathrm{d}\tau\, \mathrm{e}^{-\varepsilon\tau}\, \alpha_\tau^0(A), \qquad \forall A \in \mathfrak{L}^p(\mathscr{A}). \tag{2.3.6}$$

Corollary 2.3.4 *For all $t \geq 0$ the conductivity coefficients from Theorem 2.3.3 can be computed explicitly for the following two choices of f_k:*

(1) If $f_k \equiv 1$ then

$$\widetilde{\sigma}_\varepsilon^k[J, \rho](t) = -\mathrm{i}\,\mathrm{e}^{\varepsilon t}\, \mathcal{T}\left(J\, \frac{1}{\mathscr{L}_H^{(1)} + \varepsilon}\big(\partial_{X_k}(\rho)\big)\right). \tag{2.3.7}$$

(2) In case f_k is given by (2.1.8), then

$$\widetilde{\sigma}_\varepsilon^k[J, \rho](t) = -\mathrm{i}\,\mathrm{e}^{\varepsilon t} \int_{\mathbb{R}} \mathrm{d}\kappa\, \mathrm{e}^{\mathrm{i}\kappa t}\, \hat{f}_k(\kappa)\, \mathcal{T}\left(J\, \frac{1}{\mathscr{L}_H^{(1)} + \varepsilon + \mathrm{i}\kappa}\big(\partial_{X_k}(\rho)\big)\right). \tag{2.3.8}$$

Also this result is proven in Sect. 6.2.2. Equation (2.3.7) has been first obtained in [85, Eq. (41)] and [3, Theorem 1] in the approximation of bounded tight-binding operators where C^*-algebraic (as opposed to von Neumann algebraic) techniques have been used. The analogous formula for the magnetic Laplacian in the continuum has been derived in [7, Corollary 5.10]. A formula similar to Eq. (2.3.8) appears in [49, Eq. (3.30)].

2.4 The Adiabatic Limit and the Kubo–Středa Formula

Physically the *adiabatic limit* $\varepsilon \to 0$ means that the ramp speed at which we switch on the external, macroscopic perturbation becomes infinitesimally small compared to the time scale of the microscopic dynamics. Given that here $\rho_{\mathrm{full}}(t) \to \rho_{\mathrm{int}}(t)$ should hold in some sense, we expect that many of the details on *how* the perturbation is switched on will be washed out. In comparison, the conductivity coefficients $\sigma_k^\varepsilon[J, \rho](t)$ (or, equivalently, $\widetilde{\sigma}_\varepsilon^k[J, \rho](t)$) depend on the entire history of the system until time t. Indeed, this is the primary purpose of the adiabatic limit $\varepsilon \to 0$, it leads to a time averaging of the conductivity coefficients that averages away many details of the perturbation. While with our approach the time averaging

emerges naturally, other authors, e.g. [3, 85], had to introduce it in an *ad hoc* fashion to derive the Kubo formula. Their idea is to exploit the well-known fact that Cesàro summability implies Abel summability [88, Chap. 8, Theorem 2.3] and

$$\langle a \rangle := \lim_{T \to +\infty} \frac{1}{T} \int_0^T \mathrm{d}\tau \, a(\tau) = \lim_{\varepsilon \to 0^+} \varepsilon \int_0^{+\infty} \mathrm{d}\tau \, \mathrm{e}^{-\varepsilon \tau} \, a(\tau).$$

And writing this time average as a Laplace transform allows one to relate this expression to the resolvent of the Liouvillian via (2.3.6). In our derivation the presence of the time average in (2.3.3) can be traced back to the time integral in Eq. (2.2.14) which computes the instantaneous difference between $\rho_{\mathrm{full}}(t)$ and $\rho_{\mathrm{int}}(t)$.

In order to state the main result about the adiabatic limit let us observe that the Liouvillian $\mathscr{L}_H^{(q)}$ is a linear operator on the Banach space $\mathfrak{L}^q(\mathscr{A})$ and we are interested in computing the limit of $\mathfrak{L}^q(\mathscr{A})$ times its resolvent in ε when $\varepsilon \to 0^+$ with respect to the strong operator topology in $\mathfrak{L}^q(\mathscr{A})$. The existence of this limit is proved in Sect. 5.1.2 and the result is

$$\lim_{\varepsilon \to 0^+} \frac{\mathscr{L}_H^{(q)}}{\mathscr{L}_H^{(q)} - \varepsilon}(A) = \mathscr{P}_H^{(q)\perp}(A), \qquad A \in \mathfrak{L}^q(\mathscr{A}) \tag{2.4.1}$$

where $\mathscr{P}_H^{(q)\perp}$ is a suitable idempotent (Banach space projection) acting on $\mathfrak{L}^q(\mathscr{A})$. In the special case $q = 2$ the idempotent $\mathscr{P}_H^{(2)\perp}$ turns out to be an orthogonal projection with respect to the Hilbert structure of $\mathfrak{L}^2(\mathscr{A})$, and one has the relation $\mathscr{P}_H^{(2)\perp} := \mathbb{1}_{\mathfrak{L}^2(\mathscr{A})} - \mathscr{P}_H^{(2)}$ where $\mathscr{P}_H^{(2)}$ is the projection onto the kernel $\ker\big(\mathscr{L}_H^{(2)}\big)$.

Theorem 2.4.1 (Adiabatic limit of the Kubo formula) *Suppose Hypotheses 1–6 are satisfied, and $f_k \equiv 1$. Furthermore, assume we are given a current-type observable $J(t)$ in the sense of Definition 2.3.1 for which there exists a $Q_J \in \mathfrak{L}^q(\mathscr{A})$ such that*

$$J = \mathscr{L}_H^{(q)}(Q_J)$$

with $p^{-1} + q^{-1} = 1$. Then the adiabatic limit $\varepsilon \to 0$ of the conductivity coefficients exists, and is given by

$$\sigma^k[J, \rho] = \mathrm{i} \; \mathcal{T}\Big(\mathscr{P}_H^{(q)\perp}(Q_J) \; \partial_{X_k}(\rho)\Big). \tag{2.4.2}$$

In the special case $p = q = 2$ the last formula can be recast as

$$\sigma^k[J, \rho] = \mathrm{i} \Big\langle\!\!\Big\langle \mathscr{P}_H^{(2)\perp}(Q_J)^*, \; \partial_{X_k}(\rho) \Big\rangle\!\!\Big\rangle_{\mathfrak{L}^2} \tag{2.4.3}$$

where the Hilbert structure of $\mathfrak{L}^2(\mathscr{A})$ has been used.

The proof of this result is presented in Sect. 6.3.

The most important case considered in the physics literature is the computation of the Kubo coefficients when the initial equilibrium state is a spectral projection of the Hamiltonian $P := P(H)$ and the observable is the k-th component of the density current (2.2.1) $J := J_k^{(1)}$. In this case equation (2.3.2) can be conveniently rewritten as

$$\mathscr{J}_k^{\Phi,\varepsilon}[P](t) = \sum_{j=1}^{d} \Phi_j \, \sigma_\varepsilon^{kj}[P](t) + \mathcal{O}(\Phi^2), \qquad k = 1, \dots, d, \tag{2.4.4}$$

where $\mathscr{J}_k^{\Phi,\varepsilon}[P](t) := \mathscr{J}^{\Phi,\varepsilon}\big[J_k^{(1)}, P\big](t)$ can be interpreted as the k-th component of the macroscopic current, and the $\sigma_\varepsilon^{kj}[P](t) := \sigma_k^\varepsilon\big[J_j^{(1)}, P\big](t)$ are the components of a rank two tensor. The next result enumerates sufficient conditions under which the adiabatic limit

$$\sigma^{kj}[P] := \lim_{\varepsilon \to 0^+} \sigma_\varepsilon^{kj}[P](t), \qquad k, j = 1, \dots, d,$$

exists and *can be computed explicitly*. The quantity

$$\boldsymbol{\sigma}[P] := \big\{\sigma^{kj}[P]\big\}_{k,j=1,\dots,d}$$

is called the *conductivity tensor* and, as a matter of fact, it is the most relevant object in physical applications of LRT.

Theorem 2.4.2 (The Kubo–Středa formula) *Suppose Hypotheses 1–5 hold true. Moreover, assume that P is a spectral projection of H with respect to a bounded portion of* Spec(H) *which is also* 2*-regular in the sense of Hypothesis 6.*

Then the ε-dependent conductivity coefficients

$$\sigma_\varepsilon^{kj}[P](t) := \sigma_k^\varepsilon\big[J_j^{(1)}, P\big](t), \qquad k, j = 1, \dots, d,$$

computed through the formula (2.3.3) *are well-defined, their adiabatic limits exist and are given by the* Kubo–Středa formula

$$\sigma^{kj}[P] := \lim_{\varepsilon \to 0^+} \sigma_\varepsilon^{kj}[P](t) = +\mathrm{i} \Big\langle\!\!\Big\langle \big[P, \partial_{X_k}(P)\big]_{(2)}, \partial_{X_j}(P) \Big\rangle\!\!\Big\rangle_{\mathfrak{L}^2} \tag{2.4.5a}$$

$$= -\mathrm{i}\, \mathcal{T}\Big(P \big[\partial_{X_k}(P), \partial_{X_j}(P)\big]_{(1)}\Big) \tag{2.4.5b}$$

for each $k, j = 1, \dots, d$.

The proof of this important result is the main aim of Sect. 6.3. The symbol $[\,\cdot\,,\,\cdot\,]_{(r)}$ which appears in Eq. (2.4.5) means that the commutator takes values in the space $\mathfrak{L}^r(\mathscr{A})$; we refer to Sect. 3.3.1 for details.

2.5 Zero Temperature Limit and Topological Interpretation

We already discussed that a typical way of building initial equilibrium states associated to a Hamiltonian $H \in \mathrm{Aff}(\mathscr{A})$ is to choose suitable positive functions of H. For instance, in condensed matter problems concerning electron systems (usually in the approximation of non-interacting particles) the typical initial equilibrium states are described through the *Fermi–Dirac* distribution at *inverse temperature* $\beta > 0$ and *Fermi energy* E_{F},

$$\rho_\beta(x) := \begin{cases} \frac{1}{1+\mathrm{e}^{\beta(x-E_{\mathrm{F}})}} & \beta < \infty \\ \chi_{(-\infty,E_{\mathrm{F}}]}(x) & \beta = \infty \end{cases}.$$

Here $\chi_{(-\infty,E_{\mathrm{F}}]}(x)$ denotes the characteristic function of $(-\infty, E_{\mathrm{F}}]$, i.e. $\chi_{(-\infty,E_{\mathrm{F}}]}(x)$ is 1 if $x \leqslant E_{\mathrm{F}}$ and is 0 otherwise. The associated initial equilibrium state is given by

$$\rho_\beta := \rho_\beta(H) = \begin{cases} \frac{1}{1+\mathrm{e}^{\beta(H-E_{\mathrm{F}})}} & \beta < \infty \\ P & \beta = \infty \end{cases}$$

where $P := \chi_{(-\infty,E_{\mathrm{F}}]}(H)$ is the spectral projection of H for energies up to the Fermi energy E_{F}, and is conventionally called *Fermi projection*. Since the Fermi–Dirac distribution converges pointwise to the characteristic function of $(-\infty, E_{\mathrm{F}}]$ in the limit $\beta \to +\infty$, it follows that $\rho_\beta \to P$ with respect to the strong operator topology (SOT) of operators on the Hilbert space $\mathcal{H}$. The limit $\beta \to +\infty$ is known in condensed matter physics as the *zero temperature limit*.

Suppose $\rho_\beta = \rho_\beta(H)$ is a net of 2-regular initial equilibrium states according to Hypothesis 6 with the following two additional properties:

(iii) $\rho_\beta \to P$ in the topology of $\mathfrak{L}^1(\mathscr{A})$ where P is a 2-regular spectral projection of H, and

(iv) $H\, \partial_{X_k}(\rho_\beta) \to H\, \partial_{X_k}(P)$ in the topology of $\mathfrak{L}^1(\mathscr{A})$.

Under these conditions, in particular (iv), one has that

$$\lim_{\beta\to+\infty} \mathcal{T}\left(J\, \alpha_t^0\big(\partial_{X_k}(\rho_\beta)\big)\right) = \mathcal{T}\left(J\, \alpha_t^0\big(\partial_{X_k}(P)\big)\right)$$

and the application of the Dominated Convergence Theorem in (2.3.3) leads to

$$\lim_{\beta\to+\infty} \sigma_k^\varepsilon[J, \rho_\beta](t) = \sigma_k^\varepsilon[J, P](t).$$

The Kubo–Středa formula is the adiabatic limit of $\sigma_k^\varepsilon\big[J_j^{(1)}, P\big](t)$, and hence one has

$$\lim_{\varepsilon\to 0^+} \lim_{\beta\to+\infty} \sigma_k^\varepsilon\big[J_j^{(1)}, \rho_\beta\big](t) = \sigma^{kj}[P]$$

where $\sigma^{kj}[P]$ is given by (2.4.5). In other words, under suitable conditions (e.g. property (iv) above) the Kubo–Středa formula can be seen as the "zero temperature limit" of the Kubo formula. Let us point out that the zero temperature limit has to be taken first and *then* one computes the adiabatic limit. The two limits do not commute in general.

Let us briefly discuss one last aspect of the Kubo–Středa formula. Under appropriate circumstances the right-hand side of (2.4.5) has the structure of a 2-cocycle over a (sub) $*$-algebra contained in $\mathscr{A}$. This associates the components $\sigma^{kj}[P]$ with Chern–Connes characters which are quantities of topological nature [13, Part IV], [2, Sect. F]. The equality of the components of the conductivity tensor as given by the Kubo–Středa formula with Chern–Connes characters (up to physical proportionality constants) goes under the name of *Kubo–Chern formula*. This is the crucial ingredient in the topological interpretation of the Quantum Hall Effect via LRT [2, 85], which gave birth to the theory of *topological insulators*, one of the most active areas of condensed matter physics today. However, the geometric aspects of the Kubo–Středa formula are still quite a hot topic in many areas of condensed matter physics, and a more detailed analysis is beyond the scope of this work.

2.6 The Tight-Binding Type Simplification

For simpler systems, most notably those described by tight-binding operators, the setting for LRT can be greatly simplified [3, 85], because the assumptions avoid the main technical problems we tackle in this work.

Definition 2.6.1 (Tight-binding-type setting) *One is in a* tight-binding-type setting *if* $\mathcal{T}(\mathbb{1}) = 1$ *and* $H \in \mathscr{A}$.

The first condition, $\mathcal{T}(\mathbb{1}) = 1$, implies the trace is in fact finite (as opposed to semi-finite), and therefore $\mathrm{Aff}(\mathscr{A})$ agrees automatically with the $*$-algebra of measurable operators with respect to $\mathcal{T}$ (see Example 3.2.6 (3) and references therein). Additionally, $\mathscr{A}$ itself is contained in all of the other $\mathfrak{L}^p(\mathscr{A})$ spaces. The second condition, $H \in \mathscr{A}$, has several implications, most notably that many of the products of H with operators in $\mathfrak{L}^p(\mathscr{A})$ are unambiguously defined thanks to the $\mathscr{A}$-module structure of the $\mathfrak{L}^p(\mathscr{A})$ spaces and the Leibniz rule (see Proposition 3.4.3 (2) and related comments).

Furthermore, $H \in \mathscr{A}$ implies that many of our Hypotheses are automatically verified. Due to the boundedness we know $\mathscr{D}_{\mathrm{c}}(H) = \mathscr{D}_{\mathrm{c}}$ holds and so item (i) of Hypothesis 5 is trivially satisfied. The same goes for item (iv) of Hypothesis 5. Items (ii) and (iii) of Hypothesis 5 just say that the iterated commutators of H with the X_k's are well-defined as bounded operators, and thanks to Lemma 6.1.1 (1) we also know that these commutators have to be elements of the algebra $\mathscr{A}$.

In summary, Hypothesis 5 just states that H has to be a regular (indeed a smooth) element of $\mathscr{A}$ with respect the *spatial derivations* induced on $\mathscr{A}$ by the generators X_k's (see Definition 3.4.1 for more details). Let $\mathfrak{C}^n(\mathscr{A}) \subset \mathscr{A}$ be the subset

of elements which can be derived n-times inside the algebra (one can also write $\mathfrak{C}^n(\mathscr{A}) \equiv \mathfrak{W}^{n,\infty}(\mathscr{A})$ in agreement with the notation previously introduced). Then, in the tight-binding type setting Hypothesis 5 can be simply replaced by

Assumption 2.6.2 (Differentiability of H) *$H \in \mathfrak{C}^n(\mathscr{A})$ for a sufficiently large n (e.g. $n = \infty$) and*

$$J_\kappa = (-1)^{|\kappa|}\, \partial_X^\kappa(H) := (-1)^{|\kappa|}\, \partial_{X_1}^{\kappa_1} \circ \cdots \circ \partial_{X_d}^{\kappa_d}(H)$$

for all $\kappa \in \mathbb{N}_0^d$ with $|\kappa| \leqslant n$.

Hypothesis 6 can be simplified to the only regularity requirement (i),

$$\rho \in \mathscr{A}^+ \cap \mathfrak{W}^{1,1}(\mathscr{A}) \cap \mathfrak{W}^{1,p}(\mathscr{A}).$$

The H-regularity described by item (ii) of Hypothesis 6 just follows because the $\mathscr{A}$-module structure of the spaces $\mathfrak{L}^p(\mathscr{A})$ and the smoothness of H.

Also Hypothesis 5 is automatically satisfied, and just states that any $J \in \mathscr{A}$ is a current-type observable which is sufficiently well-behaved to derive the Kubo's formula. Finally, the extra Assumption (iv) in the statement of Theorem 2.4.1 becomes equivalent to $J = \mathrm{i}\,[Q_J, H]$ for a $Q_J \in \mathscr{A} \cap \mathfrak{L}^q(\mathscr{A})$. Finally, *any* spectral projection P of H automatically meets the requirement (iii) in the statement of Theorem 2.4.2.

In conclusion, even though problems described by tight-binding operators do not necessitate the level of generality we insist on here and avoid the main technical stumbling blocks, they are nevertheless covered by the framework we propose. We will revisit this point in Chap. 4 where we give the procedure to construct von Neumann algebra and the trace per unit volume, which applies to $\mathbb{Z}^d$ and $\mathbb{R}^d$; in Chap. 7 we will talk about specific examples of tight-binding operators.

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